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Energy Transfer in Molecular Layer-by-Layer Films of Water-Soluble Perylene Diimides

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Table S1: Experimental Φ_{ET} data and best fit comparison

n	Φ_{ET} data	PL, x=2, $d_0 = 5.9^a$	PL, x=4 $d_0 = 5.6^a$	KW model $d_0 = 6.0^a$	OL, x=2 $d_0 = 11.3^a$	OL, x=4 $d_0 = 11.5^a$
1	0.9855	0.9600	0.9979	0.9868	0.9892	0.9998
2	0.9101	0.9086	0.9831	0.9498	0.9584	0.9979
3	0.8804	0.8481	0.9412	0.8950	0.9110	0.9897
4	0.7821	0.7861	0.8699	0.8300	0.8520	0.9682
5	0.7595	0.7269	0.7836	0.7615	0.7866	0.9258
6	0.7049	0.6724	0.6986	0.6947	0.7191	0.8576
7	0.6570	0.6233	0.6229	0.6323	0.6528	0.7648
8	0.5818	0.5795	0.5583	0.5760	0.5901	0.6558
9	0.5031	0.5405	0.5040	0.5260	0.5322	0.5433
10	0.4874	0.5058	0.4582	0.4820	0.4796	0.4384
11	0.4534	0.4749	0.4195	0.4435	0.4323	0.3477
12	0.4298	0.4472	0.3865	0.4098	0.3902	0.2735

a. $d_0 = 1.2 n_0$ (nm) where n_0 is the best fit value from Table 2.

Table S2: Weighted differences $((\Phi_{ET}^{expt} - \Phi_{ET}^{calc}) / \Phi_{ET}^{expt})$

N	x=2 - expt	x=4-expt	KW-expt	OL(x=2)-expt	OL(x=4)-expt
1	0.025919475	-0.012575225	0.001334649	-0.00375883	-0.01452037
2	0.00172545	-0.080125248	0.043614689	-0.052986791	-0.09644239
3	0.036632277	-0.069102106	0.016629911	-0.034745171	-0.12413202
4	-0.005167042	-0.112272008	0.061270182	-0.089430696	-0.23797594
5	0.042913548	-0.03177088	0.002749173	-0.03569484	-0.21905783
6	0.046128967	0.009000319	-0.014541547	-0.020054505	-0.2165695
7	0.051249605	0.051881367	-0.03750079	0.006327128	-0.16402562
8	0.003882746	0.040249256	-0.009896698	-0.014374649	-0.12736056
9	-0.074392928	-0.001805628	0.045473861	-0.057838979	-0.08000303
10	-0.037780289	0.059825053	-0.011139137	0.016090392	0.10053464
11	-0.047347141	0.074764289	-0.021909397	0.046538811	0.2330085
12	-0.040593135	0.100750382	-0.046403091	0.092052721	0.36360193
Sum ^b	<u>0.003171532</u>	0.02881957	0.029681806	-0.14787541	-0.5829422
Slopes ^a	-0.007525459	0.015225003	<u>-0.005066761</u>	0.008929396	0.03431668

- Slope from least-squares linear fit to weighted differences and smallest value corresponds to the fit in which the experimental values and the fit have the least correlation with n (see plot S3) (lowest value highlighted).
- Sum of weighted differences. If the values were perfectly random then the sum should tend to zero as n increases (lowest value underlined).

Figure S3: Plot of weighted difference $((\Phi_{\text{ET}}^{\text{expt}} - \Phi_{\text{ET}}^{\text{calc}}) / \Phi_{\text{ET}}^{\text{expt}})$ vs. n (data in Table S2), illustrating the degree of correlation in different fits. The OL ($x=4$) model is excluded from this plot because of the very large values of the weighted differences.

